Positive-definite states of a Klein-Gordon type particle

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Abstract. A possible way for the consistent probability interpretation of the Klein-Gordon equation is proposed. Assuming that some states can not be physically realized, i.e. specifying the requirements of superselection rules, one obtains well-defined probability distributions for the rest quantum states. It is shown that this approach is closely related to the description of a Klein-Gordon type particle with the Newton-Wigner coordinate.

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The problem of physical interpretation of the Klein–Gordon equation has a very long history. Firstly defined by Schrödinger as a wave equation describing a relativistic quantum particle [1], it has been considered also by Klein [2], Gordon [3], and Fock [4]. However, it was impossible to give a consistent probability interpretation for solutions of this equation, because the corresponding distribution function has negative values, unlike the case of the Schrödinger equation. Later a four-component relativistic quantum wave equation, which is free of this problem, has been proposed by Dirac [5]. During some time the Dirac equation was considered as the unique possible way for the consistent formulation of relativistic quantum mechanics. In 1934 Pauli and Weisskopf [6] gave a new physical interpretation for the Klein-Gordon equation in the framework of the field-theoretical approach, which allowed to get the correct probability interpretation for measurement of some collective observables, e.g. the energy of quanta. Nowadays, the Klein-Gordon equation is used in several branches of physics. Specifically, it describes spinless particles, e.g. π-mesons, which are the carriers of the nuclear interactions. In cosmology this equation has found its application for a description of the fundamental scalar field [7, 8].

The field-theoretical approach does leave an open question about the correct definition of the probability distribution for such an observable as coordinate. Indeed, eigenstates of the standard operator of coordinate are superpositions of states with different signs of charge. Such states cannot be realized in the nature due to the fundamental charge superselection rule [9]. In 1949 Newton and Wigner proposed another operator of coordinate [10] with non-charge-violated eigenstates – an approach, which meets at least two serious problems, absence of the Lorentz-invariance, and impossibility to formulate an operational procedure for measurement of such an observable.

In the last years some different ways to resolve this problem have been proposed. First of all, one should note the consideration given by Mostafazadeh [11]. In this approach a redefinition of the scalar product for states has been introduced. This has allowed the author to define hermitian-conjugated Hamiltonian and positive defined probability distribution. This approach is very closely connected with $\mathcal{PT}$ symmetrical quantum mechanics developed recently by Bender with collaborators [12].

In this contribution we propose another way for resolving this very old problem. Our approach is based on the standard requirement that quantum states of a system can be described only by positive-definite density operator. It will be demonstrated that the most of pure states of a Klein-Gordon type particle do not obey this condition. Positive-definite states are, as rule, mixed ones. As we will see, such a restriction for the possible class of quantum states is formally equivalent to the description of a Klein-Gordon type particle in terms of the Newton-Wigner coordinate. This can be considered as a counterpart of duality between Schrödinger and Heisenberg pictures of motion. An advantage is that one may not apply any special measurement procedures for the Newton-Wigner coordinate. However the problem, related to the absence of the Lorentz invariance, is still unresolved in the proposed approach.

The point that not all possible elements of the Hilbert space can be associated with real physical states is not a new one in quantum field theory. In 1956 Wick, Wightman, and Wigner have presented superselection rules [9]. According to them some elements of the Hilbert space do not have a physical realization. For example, this is related to a superposition of states with different signs of charge (particle and antiparticle). The proposed approach introduces a stronger requirement for the possible set of physically consistent states of a scalar charged particle.

Let us start from the well-known Feshbach-Villars form of the Klein-Gordon equation [13]

$$i\hbar\partial_t\Psi = \hat{H}\Psi, \tag{1}$$

where the Hamiltonian

$$\hat{H} = (\tau_3 + i\tau_2)\,\frac{\hat{p}^2}{2m} + \tau_3 mc^2 \tag{2}$$

is 2×2 operator-valued matrix, and τ_i are the Pauli matrices. Appearance of these matrices can be considered as an introduction of a new internal degree of freedom, so-called charge variable, which is responsible for the sign of energy – subdivision on particles and antiparticles. However, the charge superselection rule restricts a class of possible physical states associated with it.

Utilizing generalized unitary transformation, which is defined by the operator-valued matrix

$$\hat{U} = \frac{1}{2\sqrt{mc^2\hat{E}}}\left[\left(\hat{E} + mc^2\right) + \left(\hat{E} - mc^2\right)\tau_1\right] \tag{3}$$

and inverted one

$$\hat{U}^{-1} = \frac{1}{2\sqrt{mc^2\hat{E}}}\left[\left(\hat{E} + mc^2\right) - \left(\hat{E} - mc^2\right)\tau_1\right], \tag{4}$$

where

$$\hat{E} = \sqrt{m^2c^4 + c^2\hat{p}^2}, \tag{5}$$

the Hamiltonian (2) can be diagonalized to the form

$$\hat{H}^{\mathrm{FV}} = \hat{U}^{-1}\hat{H}\hat{U} = \tau_3\,\hat{E}. \tag{6}$$

The corresponding representation is referred to as the Feshbach-Villars (FV) representation. An arbitrary observable $\hat{A}$ can be transformed into this representation according to the rule

$$\hat{A}^{\mathrm{FV}} = \hat{U}^{-1}\hat{A}\hat{U}. \tag{7}$$

In many problems of quantum field theory one usually deals with measurements of energy. Probability distribution for this observable is always sign-definite. However, this is not true for the other observables, such as the coordinate. Generally speaking, only the fact that eigenstates of this observable are superpositions of states with different signs of charge is not a problem for the consistent interpretation of the corresponding probability density. For example, the probability density for the standard (not Newton-Wigner) coordinate is always positive-definite for Dirac particles [14]. However, this is not the case for Klein-Gordon particles, for which the probability density may do have negative values due to the indefinite metric of the corresponding Hilbert space of states, see e.g. [15]. In what follows, we will demonstrate that for such particles there exists a class of density operators, which correspond to completely positive probability densities for the standard coordinate as well as for other observables.

Consider an observable $\hat{A}$, which is an arbitrary function of the coordinate and momentum,

$$\hat{A} = F\left(\hat{p}, \hat{q}\right). \tag{8}$$

In FV representation it can be written as follows:

$$\hat{A}^{\mathrm{FV}} = \left(\mathcal{E} - \tau_1 \mathcal{X}\right)\hat{A}. \tag{9}$$

Here $\mathcal{E}$ and $\mathcal{X}$ are superoperators, which act on $\hat{A}$ according to the following rules:

$$\langle p_2| \, \mathcal{E}\hat{A} \, |p_1\rangle = \varepsilon\left(p_2, p_1\right) \langle p_2| \, \hat{A} \, |p_1\rangle \,, \tag{10}$$

$$\langle p_2| \, \mathcal{X}\hat{A} \, |p_1\rangle = -\chi\left(p_2, p_1\right) \langle p_2| \, \hat{A} \, |p_1\rangle \,, \tag{11}$$

where the functions $\varepsilon\left(p_2, p_1\right)$ and $\chi\left(p_2, p_1\right)$ are defined as

$$\varepsilon\left(p_2, p_1\right) = \frac{E(p_2) + E(p_1)}{2\sqrt{E(p_2)E(p_1)}}, \tag{12}$$

$$\chi\left(p_2, p_1\right) = \frac{E(p_2) - E(p_1)}{2\sqrt{E(p_2)E(p_1)}}, \tag{13}$$

and $|p\rangle$, $E\left(p\right)$ are eigenstates and eigenvalues, respectively, of the operator (5). Any state of a scalar charged particle satisfies the charge superselection rule, i.e. it does not include interference terms between particle and antiparticle. Moreover, without losses of generality one can consider only a part of density operator, which is responsible for a particle with one sign of energy, e.g. positive one. This means that the expected value of the observable (8), (9) can be written down as follows

$$\bar{A} = \mathrm{Tr}\left(\hat{\varrho}\, \mathcal{E}\hat{A}\right), \tag{14}$$

where $\hat{\varrho}$ is the density operator in the FV representation. It is obvious that action of the superoperator $\mathcal{E}$ can be transferred from $\hat{A}$ to $\hat{\varrho}$ under the sign of trace in the last equation. This means that introducing an operator

$$\hat{\varrho}_{\mathcal{E}} = \mathcal{E}\hat{\varrho}, \tag{15}$$

which we refer as *effective density operator*, one can rewrite Eq. (14) as following

$$\bar{A} = \mathrm{Tr}\left(\hat{\varrho}_{\mathcal{E}}\hat{A}\right). \tag{16}$$

Note the following features:

(i) Action of the superoperator $\mathcal{E}$ on the density operator is very similar to the description of decoherence in open quantum systems [16]. The difference is that in the considered case $\varepsilon\left(p_2, p_1\right) > 1$ for $p_2 \neq p_1$.

(ii) The effective density operator $\hat{\varrho}_{\varepsilon}$ is not, generally speaking, a positive-definite one that means a possibility of existence of its negative eigenvalues.

The latter is the reason for problems in consistent probability interpretation for a Klein-Gordon type particle.

However, one can suppose that physically consistent states should be described by positive-definite effective density operators only. This means that we should consider the states only, which satisfy the following condition

$$\hat{\varrho} = \mathcal{E}^{-1}\hat{\varrho}_{\varepsilon}, \tag{17}$$

where $\hat{\varrho}_{\varepsilon}$ is an any positive-definite operator for which $\mathrm{Tr}\left(\hat{\varrho}_{\varepsilon}\right) = 1$, $\mathcal{E}^{-1}$ is the superoperator inverted to $\mathcal{E}$ and defined by means of the rule

$$\langle p_2| \mathcal{E}^{-1}\hat{\varrho}_{\varepsilon} |p_1\rangle = \varepsilon^{-1}\left(p_2, p_1\right) \langle p_2| \hat{\varrho}_{\varepsilon} |p_1\rangle \,. \tag{18}$$

Taking into account that

$$\varepsilon^{-1}\left(p_2, p_1\right) = \varepsilon^{-1}\left(p_1, p_2\right) < 1 \,\mathrm{for}\, p_2 \neq p_1 \tag{19}$$

$$\varepsilon^{-1}\left(p, p\right) = 1 \tag{20}$$

one can conclude that in general case a physically consistent state is a mixed one. Only eigenstates of the Hamiltonian are pure ones and obey the condition (17).

An example of a positive-definite state is a natural generalization of a coherent state $|\alpha\rangle$

$$\hat{\varrho}_{\alpha} = \mathcal{E}^{-1} |\alpha\rangle \langle\alpha| \,. \tag{21}$$

Contrary to the non-relativistic case (for a review see e.g. [17]) this state is not a pure one. However it manifests all classical properties, that a usual coherent state does. Note that all pure relativistic coherent states of a scalar charged particle (including those presented in [15]) are not positive-definite and do not obey the condition (17). We conclude that the charge superselection rule, presented by Wick, Wightman, and Wigner, in case of a scalar charged particle, can be specified. As a result we obtain a consistent positive-definite probability for a quite wide class of observables. Non-stationary states, which are allowed by this new rule, are mixed ones.

It is easy to see that any operator $\hat{A}$, which is defined by eq. (8), is written in terms of the Newton-Wigner coordinate $\hat{\xi}$ in the rule (16) for calculation of the expected value,

$$\hat{A} = F\left(\hat{p}, \hat{\xi}\right). \tag{22}$$

Particularly, the expected value of the standard coordinate $\hat{q}$ can be written as

$$\bar{q} = \mathrm{Tr}\left(\hat{\varrho}_{\varepsilon}\hat{\xi}\right). \tag{23}$$

Probability density to get the value q for the standard coordinate is

$$P\left(q\right) = \mathrm{Tr}\left(\hat{\varrho}_{\varepsilon} \left|\xi = q\right\rangle \left\langle \xi = q\right|\right), \tag{24}$$

where $|\xi = q\rangle$ is an eigenvector of the Newton-Wigner coordinate $\hat{\xi}$ with the eigenvalue q. More generally, since

$$\mathrm{Tr}\left[\hat{\varrho}_{\varepsilon}\, F\Big(\hat{p}, \hat{\xi}\Big)\right] = \mathrm{Tr}\left[\hat{\varrho}\, F(\hat{p}, \hat{q})\right], \tag{25}$$

one can use the Newton-Wigner coordinate $\hat{\xi}$ with the effective density operator $\hat{\varrho}_{\mathcal{E}}$ and get the same result as for the standard coordinate $\hat{q}$ with the density operator $\hat{\varrho}$.

The proposed consideration can be easily generalized to the class of observables, which are arbitrary functions of the coordinate, momentum and energy, i.e.

$$\hat{A} = F\left(\hat{p}, \hat{q}, \hat{H}\right). \tag{26}$$

In order to demonstrate it, let us firstly expand this observable in series

$$\hat{A} = \sum_{n,m,l} \hat{p}^n \hat{q}^m \hat{H}^l. \tag{27}$$

In the FV representation this expression has the form

$$\hat{A}^{\mathrm{FV}} = \sum_{n,m,l} \left(\mathcal{E} - \tau_1 \mathcal{X}\right) \hat{p}^n \hat{\xi}^m \left(\tau_3 \hat{E}\right)^l. \tag{28}$$

It now follows that the expected value of this operator can be written as

$$\bar{A} = \mathrm{Tr}\left[\hat{\varrho}\, \mathcal{E} F\left(\hat{p}, \hat{\xi}, \pm\hat{E}\right)\right], \tag{29}$$

where $\pm$ denotes the sign of charge. In terms of the effective density operator it is rewritten,

$$\bar{A} = \mathrm{Tr}\left[\hat{\varrho}_{\mathcal{E}}\, F\left(\hat{p}, \hat{\xi}, \pm\hat{E}\right)\right]. \tag{30}$$

Arguing as above, we see that for such observables one can use the same effective density operator and require its positivity.

It is worth noting that the introduction of the effective density operator allows one to consider a class of relativistic phase-space distributions, which are not matrix-valued and correctly characterize a quantum state of a Klein-Gordon type particle. Following to [18] we will present s-parameterized phase-space distribution of a scalar charged particle as

$$P\left(\alpha; s\right) = \frac{1}{\pi^2} \int\limits_{-\infty}^{+\infty} \mathrm{d}^2\beta \ \mathrm{Tr}\left[\hat{\varrho}_{\mathcal{E}}\, e^{(\hat{a}^\dagger - \alpha^*)\beta - (\hat{a} - \alpha)\beta^* + s\frac{|\beta|^2}{2}}\right], \tag{31}$$

where $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation operators, which are the standard complexification of the Newton-Wigner coordinate and the momentum operators. For $s = 0$ this is the relativistic Wigner function considered in [19], for $s = 1$ this is the relativistic Glauber-Sudarshan distribution, for $s = -1$ this is the relativistic Husimi-Kano distribution.

In conclusion we note, that the specification of the superselection rule results in the correct definition of the probability density for a wide enough class of observables. Particularly, this is related to the coordinate, momentum, and energy. This approach does not require redefinitions of the basic quantum mechanical and quantum field theory notions. Introduction of the effective density operators allows one to formulate operational procedures for the measurement of realistic observables, such as the standard coordinate and, at the same time, to consider well-defined probability distribution for such an observable as the Newton-Wigner coordinate. However, the proposed approach has a common disadvantage with the Newton-Wigner coordinate – absence of the Lorentz invariance. Consequently, a state, which is positive-definite in a given reference frame, may not have such a property in another one. In this connection one may formulate the problem of the "global" positivity – whether can one point out on a class of density operators, which are positive-definite in all reference frames?

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